

# Higher-order mutual information and statistical correlations in a one-dimensional quantum well

V.S. Yépez,<sup>1</sup> R.P. Sagar,<sup>1</sup> and H.G. Laguna<sup>1,2</sup>

<sup>1</sup>*Departamento de Química, Universidad Autónoma Metropolitana, San Rafael Atlixco No. 186, Iztapalapa, 09340, Ciudad de México, México.*

<sup>2</sup>*Departamento de Matemáticas, Facultad de Ciencias; y Centro de Ciencias de la Complejidad, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, Ciudad de México, 04510, México.*

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The influence of wave function symmetry on statistical correlation is studied for the case of three non-interacting spin-free quantum particles in a unidimensional box, in position and in momentum space. Higher-order statistical correlations occurring among the particles in this three-particle quantum system is quantified via higher-order mutual information and compared to the correlation between pairs of variables in this model, and to the correlation in the two-particle system. The results for the higher-order mutual information show that in general symmetric wave functions are more correlated than the antisymmetric ones with same quantum numbers. This holds in position as well as in momentum space. This behavior is opposite to that observed for the correlation between pairs of variables in this model, and the two-particle system, where the antisymmetric wave functions are in general more correlated. The use of higher-order mutual information as a correlation measure, is monitored and examined by considering a superposition of states or systems with two Slater determinants.

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## I. INTRODUCTION

The study of the effects of indistinguishability on the statistical correlation between particles in quantum systems emanates from the need to understand the characteristics that the wave functions present in such systems<sup>1-7</sup>. An understanding of how wave function properties influence the correlation among quantum particles is important for understanding quantum phenomena, especially important when addressing the present and future miniaturization of technological devices.

The symmetrization of wave functions arising from the indistinguishability requirement they must fulfill is a source of correlation between positions or momenta of the particles involved since the wave function cannot be written in a separable form. This type of correlation is distinct from the correlation that arises from a superposition of states as we shall examine in the last section.

The concept of examining correlation via the statistical correlation, in electronic quantum systems, was introduced into the literature<sup>8</sup> and has been examined via the correlation coefficient<sup>9</sup>. Our interests lie in determining the role of statistical correlation due to wave function symmetry in the distribution functions in position and in momentum space. In this work, we study the statistical correlation in the three-particle in a box system, to examine differences between symmetric and antisymmetric wave functions which for these spinless systems would be analogs of bosonic and fermionic wave functions. We first examine the correlation between pairs in the reduced distributions. Secondly, and most importantly, we then analyze the correlation among the three variables or particles by examining the higher-order mutual information and related measures.

Symmetric and antisymmetric wave functions for this three-particle spinless non-interacting system can be built from orbitals which are solutions to the one-particle in a box system of length  $L$ .

In position space, these orbitals are

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad 0 \leq x \leq L. \quad (1)$$

The corresponding orbitals in momentum space<sup>10</sup> are obtained using the Dirac-Fourier transform (with  $\hbar = 1$ ),

$$\phi_n(p) = \sqrt{\frac{1}{2\pi}} \int_0^L \psi_n(x) e^{-ipx} dx \quad -\infty \leq p \leq \infty$$

$$=(-i)\sqrt{\frac{L}{\pi}}e^{-ipL/2}\left[e^{in\pi/2\frac{\sin[(pL-n\pi)/2]}{(pL-n\pi)}}-e^{-in\pi/2\frac{\sin[(pL+n\pi)/2]}{(pL+n\pi)}}\right]. \quad (2)$$

Wave functions in position or in momentum space can be built from these orbitals using permanents (symmetric) or Slater determinants (antisymmetric) as

$$\begin{aligned} \Psi_{n_1,n_2,n_3}(x_1,x_2,x_3) &= \frac{1}{\sqrt{6}} |\psi_{n_1}(x_1) \psi_{n_2}(x_2) \psi_{n_3}(x_3)| \\ \Phi_{n_1,n_2,n_3}(p_1,p_2,p_3) &= \frac{1}{\sqrt{6}} |\phi_{n_1}(p_1) \phi_{n_2}(p_2) \phi_{n_3}(p_3)|. \end{aligned} \quad (3)$$

For symmetric functions or permanents with the three particles in the same one-particle state one has to divide by  $\sqrt{6}$  while for two particles in the same one-particle state one divides by  $\sqrt{2}$  to correctly normalize the wave function.

The particle in a box is a simple model but has wide application. For example, in the modeling of electrons in conjugated molecules<sup>11</sup>, the behavior of electrons in metals and serves as a model in the design of devices such as quantum wells.

Information theory applied to the study of quantum systems offers the possibility of gaining insights into the behavior of quantum systems. This theory provides measures of uncertainty and correlation known as the Shannon entropy and mutual information. The Shannon entropy<sup>12</sup> has been applied to study the uncertainty in the particle in a box model in position and in momentum space<sup>13–16</sup>. The study of Shannon entropies in quantum systems is of current interest<sup>17–25</sup>.

## II. SHANNON ENTROPIES

The Shannon information entropy is defined in position or in momentum space as

$$s_x = - \int \rho(x) \ln \rho(x) dx \quad s_p = - \int \pi(p) \ln \pi(p) dp, \quad (4)$$

where  $\rho(x)$  and  $\pi(p)$  are the respective position and momentum space one-particle (variable) densities normalized to unity. In one-particle systems, these densities are the squared moduli of the wave functions while for  $N$ -particle systems they are the reduced densities obtained by integration over  $N-1$  variables. All integrals in position space are over the  $[0, L]$  interval, while in momentum space they are over  $[-\infty, \infty]$ , as seen in Eqs. (1) and (2).

The interest in the Shannon entropies of both position and momentum space stems from the existence of the entropic uncertainty relationship<sup>26</sup>

$$s_x + s_p \geq 1 + \ln \pi. \quad (5)$$

The entropic uncertainty relationship has been shown to be superior to the one based on standard deviations<sup>27–30</sup>. The entropy sum,  $s_x + s_p$ , can be interpreted as the Shannon entropy of a separable phase-space distribution,  $\rho(x)\pi(p)$ .

Two-particle or pair Shannon entropies can also be considered in  $N$ -particle systems. These are defined as

$$s_\Gamma = - \int \Gamma(x_1, x_2) \ln \Gamma(x_1, x_2) dx_1 dx_2 \quad s_\Pi = - \int \Pi(p_1, p_2) \ln \Pi(p_1, p_2) dp_1 dp_2 \quad (6)$$

where  $\Gamma(x_1, x_2)$  and  $\Pi(p_1, p_2)$  are the two-particle densities in position and in momentum space, normalized to unity. In two-particle systems, these are the squared moduli of the wave functions while for three or more particle systems, they are reduced densities.

In the case of three-particle systems, such as the ones of interest here, three-particle Shannon entropies can be defined in terms of the wave functions as

$$\begin{aligned} s_\Psi &= - \int |\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2 \ln |\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2 dx_1 dx_2 dx_3 \\ s_\Phi &= - \int |\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2 \ln |\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2 dp_1 dp_2 dp_3. \end{aligned} \quad (7)$$

In systems with more than three particles, the squared moduli of the wave functions would be replaced with reduced densities in the above expressions.

The Shannon entropies at each level are measures of the uncertainties in the underlying distributions. These measures increase as the densities delocalize and decrease as the densities localize or the uncertainty diminishes. There are other measures that have been employed to measure uncertainty. Our interest in the Shannon entropies lie in their connection to measures of statistical correlation as we shall see in the next section. We emphasize that these uncertainty measures do not quantify uncertainty over states but rather the spatial uncertainty in position or in momentum space.

### III. MUTUAL INFORMATION

The interest in the one- and two-particle (variable) Shannon entropies is that they form the basis of the definition of mutual information<sup>31</sup>. In position and in momentum space

these are<sup>32,33</sup>

$$\begin{aligned} I_x &= \int \Gamma(x_1, x_2) \ln \left[ \frac{\Gamma(x_1, x_2)}{\rho(x_1)\rho(x_2)} \right] dx_1 dx_2 = 2s_x - s_\Gamma \geq 0 \\ I_p &= \int \Pi(p_1, p_2) \ln \left[ \frac{\Pi(p_1, p_2)}{\pi(p_1)\pi(p_2)} \right] dp_1 dp_2 = 2s_p - s_\Pi \geq 0. \end{aligned} \quad (8)$$

For the three-particle systems under consideration here,  $\Gamma(x_1, x_2)$  and  $\Pi(p_1, p_2)$  are the two-particle reduced densities

$$\begin{aligned} \Gamma(x_1, x_2) &= \Gamma_{n_1, n_2, n_3}(x_1, x_2) = \int |\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2 dx_3 \\ \Pi(p_1, p_2) &= \Pi_{n_1, n_2, n_3}(p_1, p_2) = \int |\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2 dp_3. \end{aligned} \quad (9)$$

Note that since the particles are indistinguishable, the integration can be performed over any one of the three variables. Furthermore, these reduced densities depend on all three quantum numbers, as shown above.

The one-particle (variable) reduced densities are similarly defined as

$$\rho(x) = \rho_{n_1, n_2, n_3}(x) = \int \Gamma(x, x_2) dx_2, \quad \pi(p) = \pi_{n_1, n_2, n_3}(p) = \int \Pi(p, p_2) dp_2 \quad (10)$$

where we have dropped the superscript on variable one to emphasize the indistinguishability. Again these reduced densities depend on  $n_1$ ,  $n_2$  and  $n_3$ .

Mutual information is a measure of the statistical correlation or dependency between pairs of variables. It is zero for independent variables or distributions that are separable and increases as the dependency between variables increases. It is a more general measure of correlation than the correlation coefficient which is only able to detect linear dependencies. This has been observed in applications to quantum systems<sup>34</sup>.

The effects of wave function symmetry on the statistical correlation between particles has been discussed in the case of two particles in a box<sup>35</sup>. Systems where the particles interact via harmonic potentials have also been examined<sup>36,37</sup>. The results obtained showed that the antisymmetric wave functions were in general more correlated than the symmetric ones<sup>35</sup> with the same quantum numbers. Furthermore, the mutual information between pairs of variables was shown to be capable of detecting correlation in cases where the correlation coefficient yielded values of zero for the linear correlation. One goal of the present work is to determine how the correlation patterns change with the addition of more particles to the system.

#### IV. MUTUAL INFORMATION WITH THREE VARIABLES

In systems with three particles or variables, there are several definitions that can be used where the correlation in the system is partitioned differently. First, one can define in each space

$$I_{3x} = \int |\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2 \ln \left[ \frac{|\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2}{\rho(x_1)\rho(x_2)\rho(x_3)} \right] dx_1 dx_2 dx_3 = 3s_x - s_\Psi \quad (11)$$

$$I_{3p} = \int |\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2 \ln \left[ \frac{|\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2}{\pi(p_1)\pi(p_2)\pi(p_3)} \right] dp_1 dp_2 dp_3 = 3s_p - s_\Phi. \quad (12)$$

These quantities measure the total correlations in the three variable system and include all correlations between pairs as well as the correlation shared among all three variables.

Another definition that can be used is<sup>37</sup>

$$I_{\rho, \Gamma} = \int |\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2 \ln \left[ \frac{|\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2}{\rho(x_1)\Gamma(x_2, x_3)} \right] dx_1 dx_2 dx_3 = s_x + s_\Gamma - s_\Psi \quad (13)$$

$$I_{\pi, \Pi} = \int |\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2 \ln \left[ \frac{|\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2}{\pi(p_1)\Pi(p_1, p_2)} \right] dp_1 dp_2 dp_3 = s_p + s_\Pi - s_\Phi. \quad (14)$$

This quantity can be interpreted as measuring the correlation between one variable (particle) and a pair of variables.

Likewise,

$$I_{\Gamma, \Gamma} = \int |\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2 \ln \left[ \frac{|\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2 \rho(x_1)}{\Gamma(x_1, x_2)\Gamma(x_1, x_3)} \right] dx_1 dx_2 dx_3 = 2s_\Gamma - s_x - s_\Psi \quad (15)$$

$$I_{\Pi, \Pi} = \int |\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2 \ln \left[ \frac{|\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2 \pi(p_1)}{\Pi(p_1, p_2)\Pi(p_1, p_3)} \right] dp_1 dp_2 dp_3 = 2s_\Pi - s_p - s_\Phi. \quad (16)$$

measures the correlation between pairs of variables.

## A. Higher-order mutual information

Perhaps of greatest interest is a measure which is capable of detecting higher-order correlation or the dependency among the three variables as a group. One can define a higher-order mutual information<sup>31,38–41</sup> as

$$I_x^3 = \int |\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2 \ln \left[ \frac{|\Psi_{n_1, n_2, n_3}(x_1, x_2, x_3)|^2 \rho(x_1) \rho(x_2) \rho(x_3)}{\Gamma(x_1, x_2) \Gamma(x_1, x_3) \Gamma(x_2, x_3)} \right] dx_1 dx_2 dx_3 \\ = 3s_\Gamma - 3s_x - s_\Psi \quad (17)$$

$$I_p^3 = \int |\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2 \ln \left[ \frac{|\Phi_{n_1, n_2, n_3}(p_1, p_2, p_3)|^2 \pi(p_1) \pi(p_2) \pi(p_3)}{\Pi(p_1, p_2) \Pi(p_1, p_3) \Pi(p_2, p_3)} \right] dp_1 dp_2 dp_3 \\ = 3s_\Pi - 3s_p - s_\Phi. \quad (18)$$

These expressions do not include a minus sign in the definition, as used elsewhere<sup>38,39</sup>, since it is closer to the definition of the pair mutual information.

Note that the second equality in the above expressions, and also those of the other previous mutual information measures, are a consequence of the indistinguishability requirements of quantum systems. For example, Eq. (17) would be

$$I_x^3 = s_{\Gamma_{x_1, x_2}} + s_{\Gamma_{x_1, x_3}} + s_{\Gamma_{x_2, x_3}} - [s_{x_1} + s_{x_2} + s_{x_3} + s_\Psi] \quad (19)$$

for a distinguishable system.

One can also establish a hierarchy among the mutual information measures with three variables and the higher-order mutual information. The differences between Eqs. (11) and (13), Eqs. (13) and (15) and Eqs. (15) and (17), are all equal to  $I_x$ , which is greater than or equal to zero. Thus

$$I_{3x} \geq I_{\rho, \Gamma} \geq I_{\Gamma, \Gamma} \geq I_x^3. \quad (20)$$

In a similar fashion in momentum space,

$$I_{3p} \geq I_{\pi, \Pi} \geq I_{\Pi, \Pi} \geq I_p^3. \quad (21)$$

The higher-order mutual information goes beyond what is captured between pairs and measures the correlation or dependency among the three variables. On the other hand, it can be negative<sup>31</sup>, unlike the mutual information between pairs of variables. Much less work has been done on higher-order mutual information as compared to the pair mutual information which has seen wide application in a variety of scientific disciplines. Also lacking is a full

understanding and interpretation of the sign of higher-order mutual information. Mutual information measures are given in natural units or nats since the units of the densities in the numerator and denominator of the logarithmic argument cancel.

One could also consider measuring correlation by extending the concept of the correlation coefficient to a  $3 \times 3$  covariance or correlation matrix for these three-variable systems. In general, these are symmetric matrices with elements  $\sigma_{ij} = \sigma_{ji}$ . In these systems with particle indistinguishability, not only would the matrices be symmetric, but each element would also be equal to all others. We did not pursue this avenue since it is not transparent how higher-order correlations could be obtained from these matrices.

Furthermore, the third-order cumulants, defined as  $C_x = \langle x_1 x_2 x_3 \rangle - 3\langle x_i x_j \rangle \langle x \rangle + 2\langle x \rangle^3$  and  $C_p = \langle p_1 p_2 p_3 \rangle - 3\langle p_i p_j \rangle \langle p \rangle + 2\langle p \rangle^3$ , for indistinguishable particles, yield a value of zero in all cases. Thus the third-order cumulant is unable to quantify the higher-order correlation.

## V. RESULTS AND DISCUSSION

Information measures were calculated from the wave functions in Eq. (3) with  $n_1, n_2, n_3 = 1 - 10$ . The box length was fixed at  $L = 1$ . The entropies, which form the basis of the information measures, were calculated by one, two and three dimensional integrations using the Mathematica<sup>42</sup> package. The numerical values were checked against those generated from quadrature routines in FORTRAN. The results for the information measures are presented by choosing  $n_1 = 1$ ,  $n_2 = 2$  and varying the value of  $n_3$ .

### A. Probability Densities

The expressions for the two-particle (variable) reduced densities are

$$\begin{aligned} \Gamma(x_1, x_2) &= \frac{1}{6} \left[ \sum_{i,j=1, i \neq j}^3 |\psi_{n_i}(x_1)|^2 |\psi_{n_j}(x_2)|^2 \pm \sum_{i,j=1, i \neq j}^3 \psi_{n_i}^*(x_1) \psi_{n_j}^*(x_2) \psi_{n_j}(x_1) \psi_{n_i}(x_2) \right] \\ \Pi(p_1, p_2) &= \frac{1}{6} \left[ \sum_{i,j=1, i \neq j}^3 |\phi_{n_i}(p_1)|^2 |\phi_{n_j}(p_2)|^2 \pm \sum_{i,j=1, i \neq j}^3 \phi_{n_i}^*(p_1) \phi_{n_j}^*(p_2) \phi_{n_j}(p_1) \phi_{n_i}(p_2) \right] \end{aligned} \quad (22)$$

where the first summation includes the Hartree-like terms while the second the exchange terms. The  $\pm$  corresponds to symmetric and antisymmetric wave functions respectively.

We present in Figures 1 and 2 the marginal or two-particle reduced density distributions in position and in momentum space,  $\Gamma(x_1, x_2)$  and  $\Pi(p_1, p_2)$ , for the symmetric and antisym-



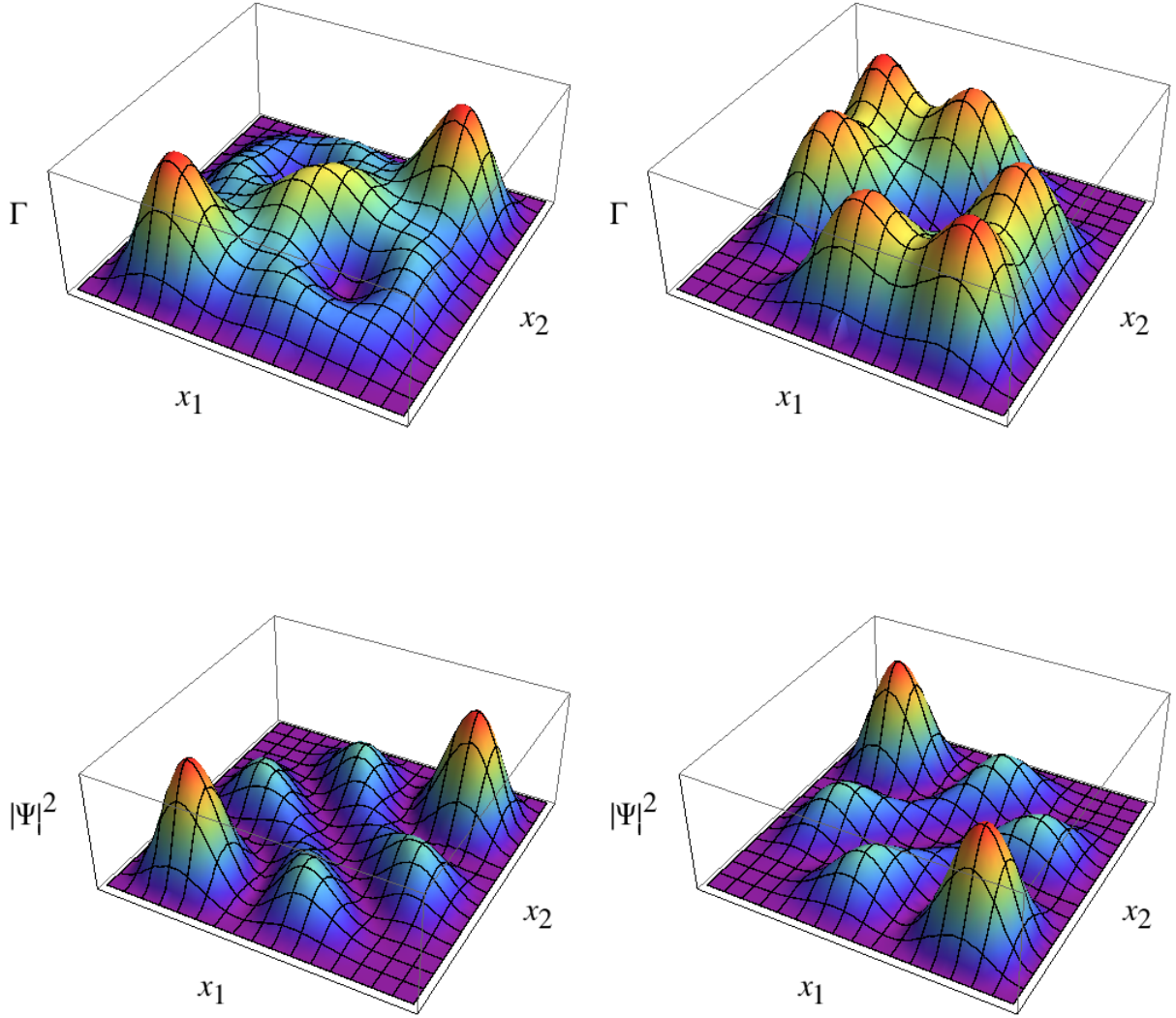


FIG. 1. Two-particle reduced densities in position space,  $\Gamma(x_1, x_2)$  (top), with  $(n_1, n_2, n_3) = (1, 2, 3)$  and  $L = 1$  for symmetric (left) and antisymmetric (right) wave functions. The densities of the two-particle system,  $|\Psi(x_1, x_2)|^2$  (bottom), with  $(n_1, n_2) = (2, 3)$  and  $L = 1$  for symmetric (left) and antisymmetric (right) wave functions, are also shown.

metric wave functions. Also presented are two-particle densities,  $|\Psi(x_1, x_2)|^2$  and  $|\Phi(p_1, p_2)|^2$  of the two-particle systems. The Fermi hole, where the density is zero when  $x_1 = x_2$  and  $p_1 = p_2$ , is clearly present in the reduced distributions of the antisymmetric function. On the other hand, there is no such hole in the densities of the symmetric function.

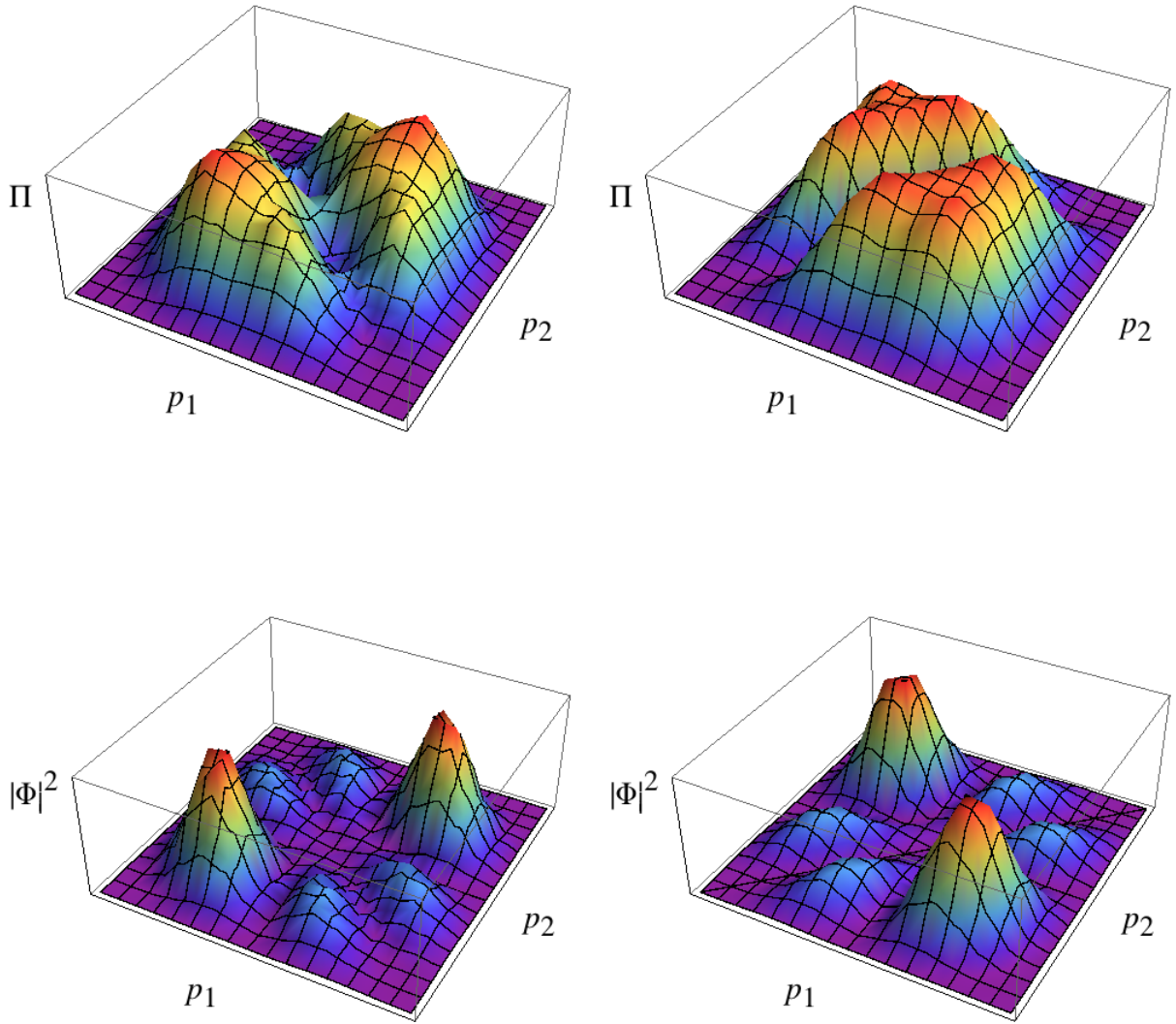


FIG. 2. Two-particle reduced densities in momentum space,  $\Pi(p_1, p_2)$  (top), with  $(n_1, n_2, n_3) = (1, 2, 3)$  and  $L = 1$  for symmetric (left) and antisymmetric (right) wave functions. The densities of the two-particle system,  $|\Phi(p_1, p_2)|^2$  (bottom), with  $(n_1, n_2) = (2, 3)$  and  $L = 1$  for symmetric (left) and antisymmetric (right) wave functions, are also shown.

This situation can be compared and contrasted to the densities of the two-particle system below where the presence of the Fermi hole is observed in the antisymmetric function. There is also another symmetry hole in the symmetric function where the density is zero when  $x_2 = 1 - x_1$ . This symmetry hole is due to the spatial symmetry of this system and not a

result of the imposed indistinguishability. This leads to equal values of two-particle entropies in the symmetric and antisymmetric functions when one quantum number is even and the other is odd. As a consequence, their pair mutual information is the same<sup>35</sup>. Counterbalance holes which can also be present in symmetric wave functions have been reported and studied in atomic systems<sup>43,44</sup>.

This behavior is different from the three-particle system where the act of reducing (integrating over a variable) the density removes the presence of the symmetry hole. We did not find any states for the three-particle system in which their two-particle entropies are equal for the symmetric and antisymmetric functions. Furthermore, we did not find any states where the three-particle entropies of the symmetric and antisymmetric functions are equal.

One-particle (variable) reduced densities are not presented because they are the same for the symmetric and antisymmetric functions in the two-particle system<sup>35</sup>, and in these three-particle systems. These are

$$\rho(x) = \frac{1}{3} \sum_{i=1}^3 |\psi_{n_i}(x)|^2 \quad \pi(p) = \frac{1}{3} \sum_{i=1}^3 |\phi_{n_i}(p)|^2. \quad (23)$$

Thus, symmetric and antisymmetric functions with the same quantum numbers have the same values of one-particle Shannon entropies. We do not present contour plots for the three-particle densities since it is difficult to visually ascertain differences between the functions.

## B. Mutual Information with two variables

The mutual information between pairs of variables (Eq. (8)) is presented in Figures 3 and 4 for symmetric and antisymmetric functions in position and in momentum space.

It is clear that the value of mutual information and hence the statistical correlation, is larger for the antisymmetric functions as compared to the symmetric ones with same quantum numbers, as expected. This is due to the presence of the Fermi hole in the two-particle reduced distributions of the antisymmetric functions and the lack of a corresponding symmetry hole in the symmetric ones, as in the case of the two-particle systems when both quantum numbers have the same parity. These results also hold for all the studied cases with other choices of quantum numbers.

There are some differences between the position and momentum space behaviors. First, mutual information increases with  $n_3$  in momentum space while it decreases (antisymmetric)

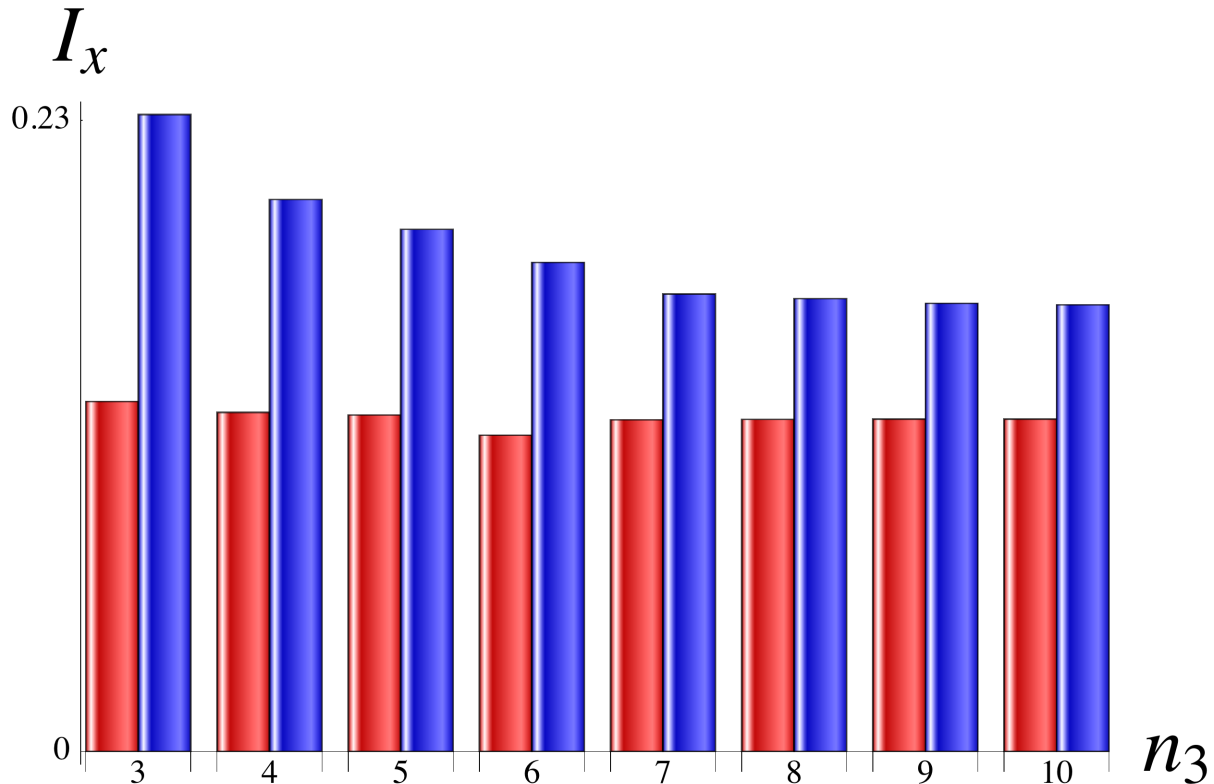


FIG. 3. Two-variable or pair mutual information,  $I_x$ , in position space for symmetric (red) and antisymmetric (blue) functions, varying  $n_3$  with  $n_1 = 1$ ,  $n_2 = 2$  and  $L = 1$ . Color online.

or slowly varies (symmetric) in position space. Secondly, the difference between the values of the two types of functions decreases in both position and momentum space as  $n_3$  increases.

Comparing the previous two figures, one notes that both types of functions are more correlated in momentum space as compared to position space ( $I_p > I_x$ ), with the exception of the antisymmetric function when  $n_3 = 3$ .

### C. Mutual Information with three variables

Mutual information between the three variables from Eqs. (11) and (12) are presented in Figures 5 and 6 for position and momentum space. We do not present figures for the two other three-variable measures (Eqs. (13) - (16)) for the sake of brevity. The general trends observed in Figures 5 and 6 are characteristic of the other measures.

The behavior in Figures 5 and 6 is very similar to that observed between the pairs in Figures 3 and 4. That is, the antisymmetric functions are more correlated than the

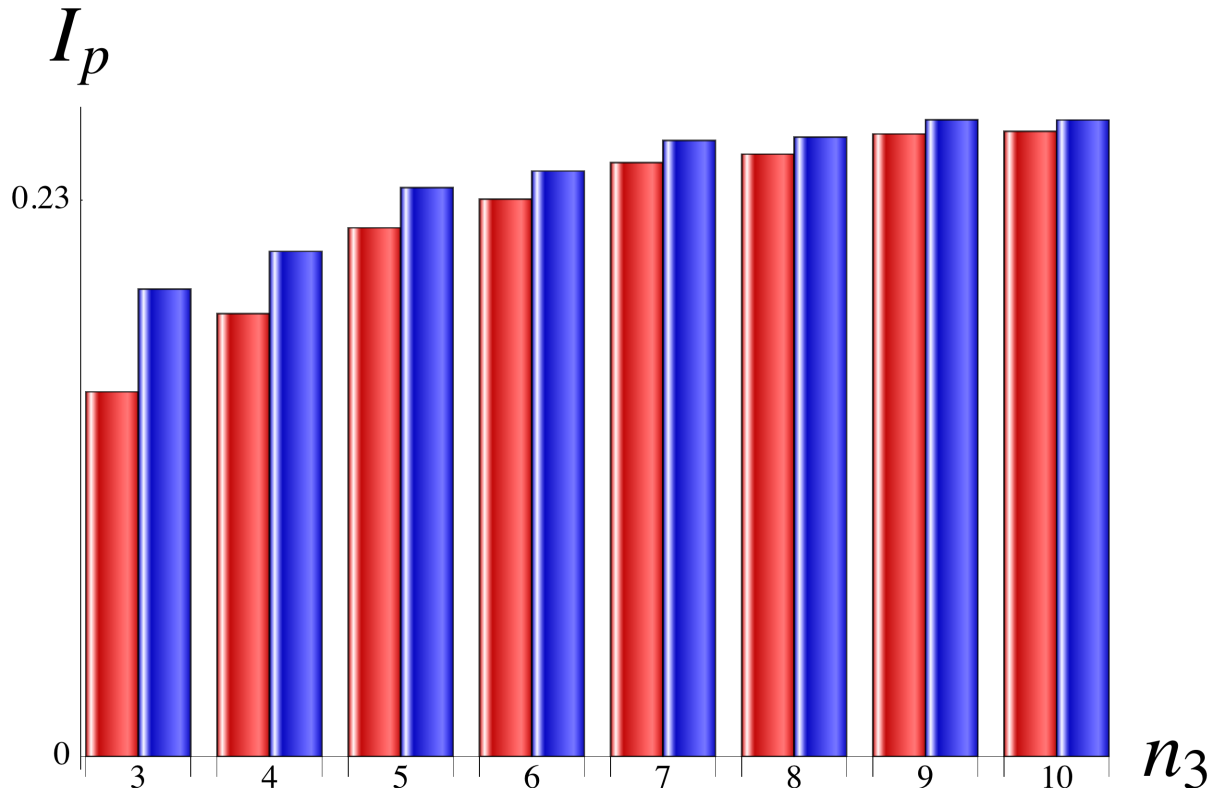


FIG. 4. Two-variable or pair mutual information,  $I_p$ , in momentum space for symmetric (red) and antisymmetric (blue) functions, varying  $n_3$  with  $n_1 = 1$ ,  $n_2 = 2$  and  $L = 1$ . Color online.

symmetric ones. This is consistent with the presence of the Fermi hole in the antisymmetric functions, and the lack of a symmetry hole in the symmetric ones.

The difference between the two types of functions is smaller in momentum space as compared to position space. Correlation increases with  $n_3$  in momentum space while it decreases or slowly varies in position space.

Similar to the behavior observed for the pair correlations,  $I_{3p} > I_{3x}$ , for both types of functions with the exception of the  $n_3 = 3$  antisymmetric state.

#### D. Higher-order mutual information

Plots of the higher-order mutual information (Eqs. (17) and (18)) in position and momentum space are presented in Figures 7 and 8.

These figures illustrate that it is now the symmetric functions which are more correlated than the antisymmetric ones in both spaces. This behavior is different to that observed be-

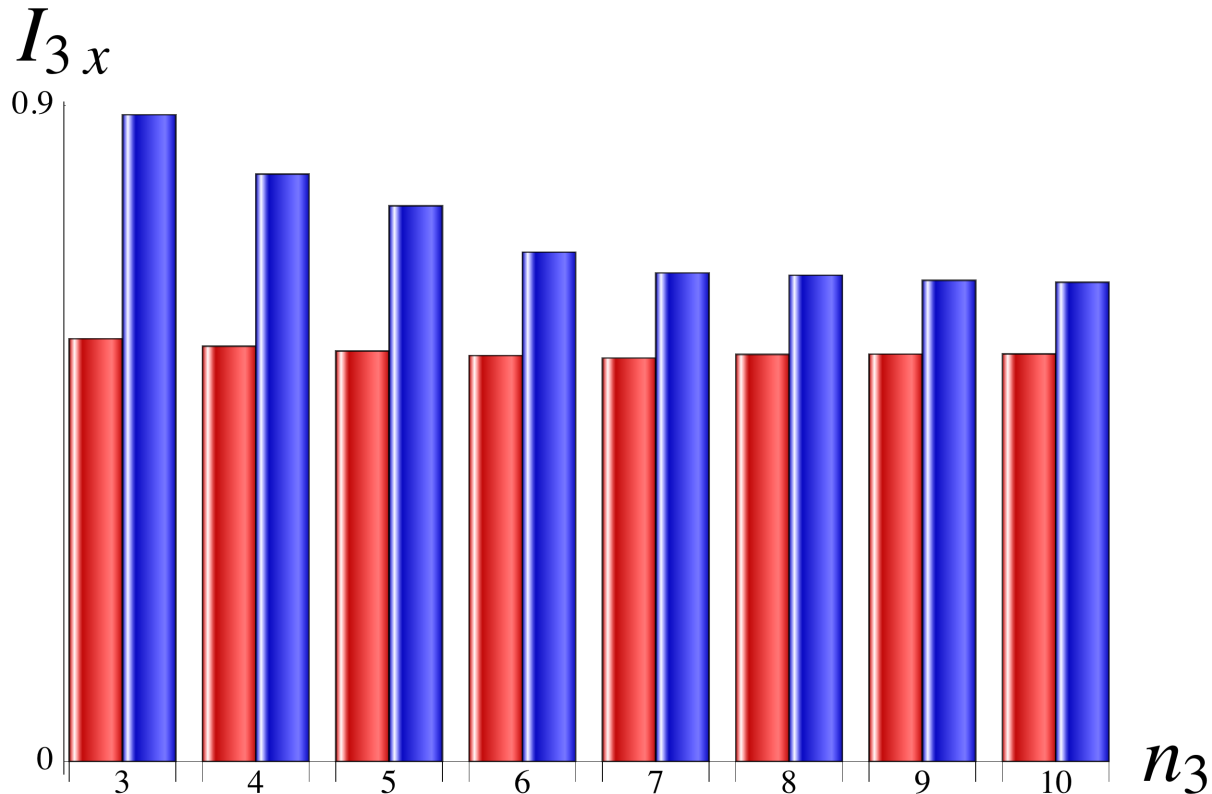


FIG. 5. Three-variable mutual information,  $I_{3x}$ , in position space for symmetric (red) and anti-symmetric (blue) functions, varying  $n_3$  with  $n_1 = 1$ ,  $n_2 = 2$  and  $L = 1$ . Color online.

tween pairs of variables and the three-variable mutual information where the antisymmetric functions are more correlated. The only deviation from this trend occurs for the  $n_3 = 4$  state in both position and momentum spaces.

However, the behavior of higher-order mutual information is similar to the other measures in that the magnitude of the correlation increases with  $n_3$  in momentum space and the differences between the two types of functions decrease with  $n_3$ . This is different from position space where the differences between the two types of functions is more marked as  $n_3$  increases.

Comparing the magnitudes of the correlation in both spaces, one observes that there is larger correlation in position space up to  $n_3 = 4$  for the symmetric functions and  $n_3 = 5$  for the antisymmetric functions. For larger  $n_3$ , there is more correlation in momentum space.

Plots of the three-particle Shannon entropies are not presented for the sake of brevity. They show in all cases that the value of the Shannon entropies is smaller for the antisymmetric functions as compared to the corresponding symmetric ones with the same quantum

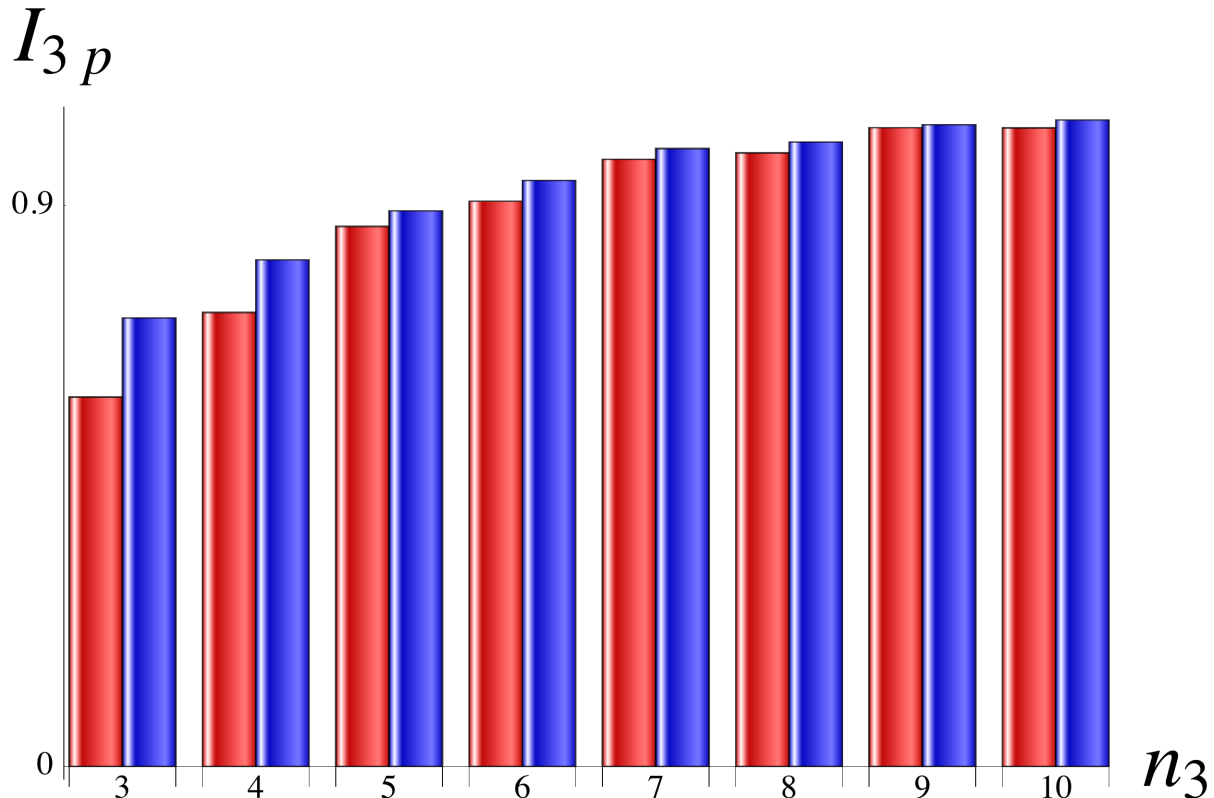


FIG. 6. Three-variable mutual information,  $I_{3p}$ , in momentum space for symmetric (red) and antisymmetric (blue) functions, varying  $n_3$  with  $n_1 = 1$ ,  $n_2 = 2$  and  $L = 1$ . Color online.

numbers. The interpretation is that the three-particle densities of the antisymmetric functions are more localized than the symmetric ones. This behavior holds for position as well as momentum space. Furthermore, this behavior was also observed for the two-particle entropies. That is, the reduced two-particle densities from the antisymmetric functions are more localized than the symmetric ones.

Note that although the behavior of all entropies is consistent with the presence of the Fermi hole in the antisymmetric functions, the combination of these entropies to form the higher-order mutual information, through Eqs. (17) and (18), yields that the symmetric functions are more correlated. Furthermore, any differences in the higher-order mutual information are a result of differences between two and three-particle Shannon entropies since one-particle entropies are equal for both types of functions.

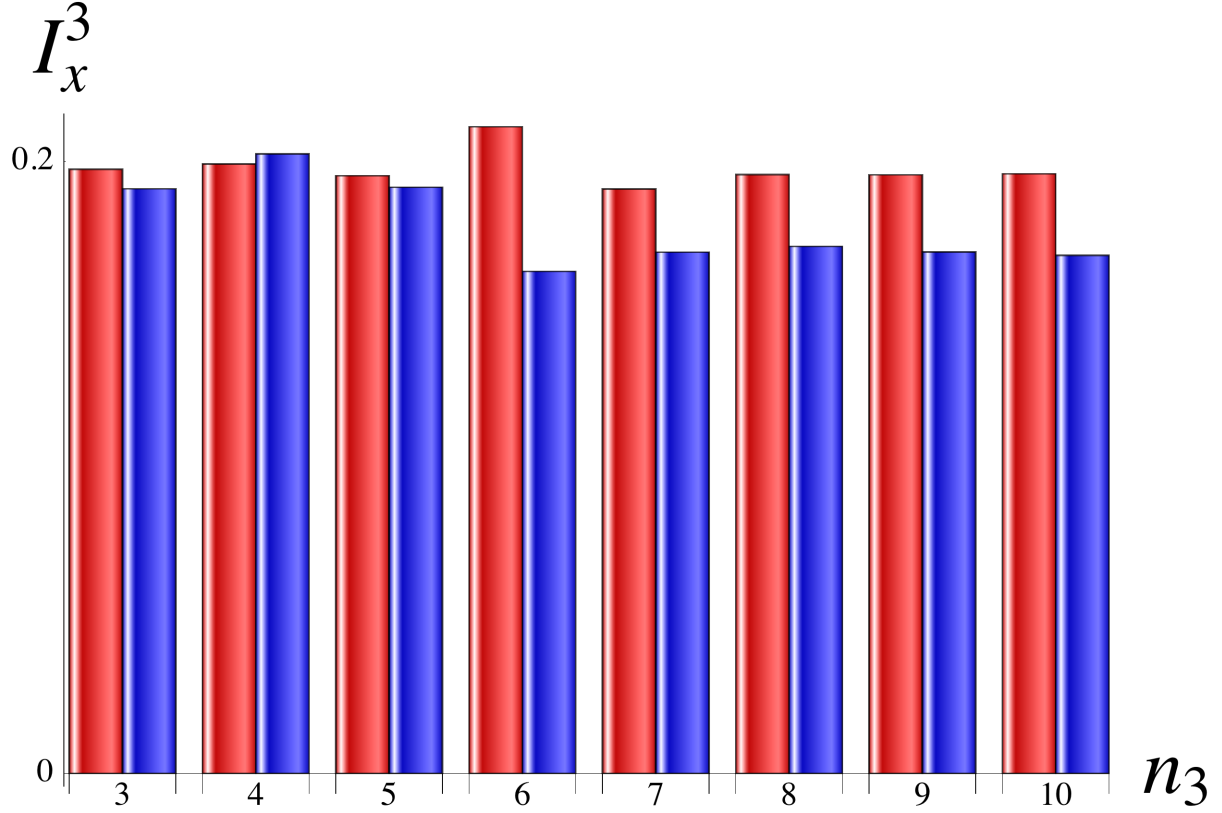


FIG. 7. Higher-order mutual information,  $I_x^3$ , in position space for symmetric (red) and antisymmetric (blue) functions, varying  $n_3$  with  $n_1 = 1$ ,  $n_2 = 2$  and  $L = 1$ . Color online.

## VI. SUPERPOSITION OF STATES

In this section, we analyze the behavior of higher-order mutual information as a correlation measure. In order to do this, one requires a model where correlation can be adjusted in a systematic manner to gauge its effect on the measure. In the absence of potentials, one can conceive of introducing correlation via the use of a superposition of states. The corresponding function in position space is

$$\Psi_S(x_1, x_2, x_3) = c_1 \Psi_{n_1, n_2, n_3}(x_1, x_2, x_3) + c_2 \Psi_{n_4, n_5, n_6}(x_1, x_2, x_3). \quad (24)$$

The three-particle density,  $|\Psi_S(x_1, x_2, x_3)|^2$ , can then be used to calculate the three-particle Shannon entropy, and reduced by integration, to obtain reduced or marginal densities from which the reduced Shannon entropies can be calculated. These expressions have been given above.

In such functions, a further source of correlation beyond the indistinguishability, is the



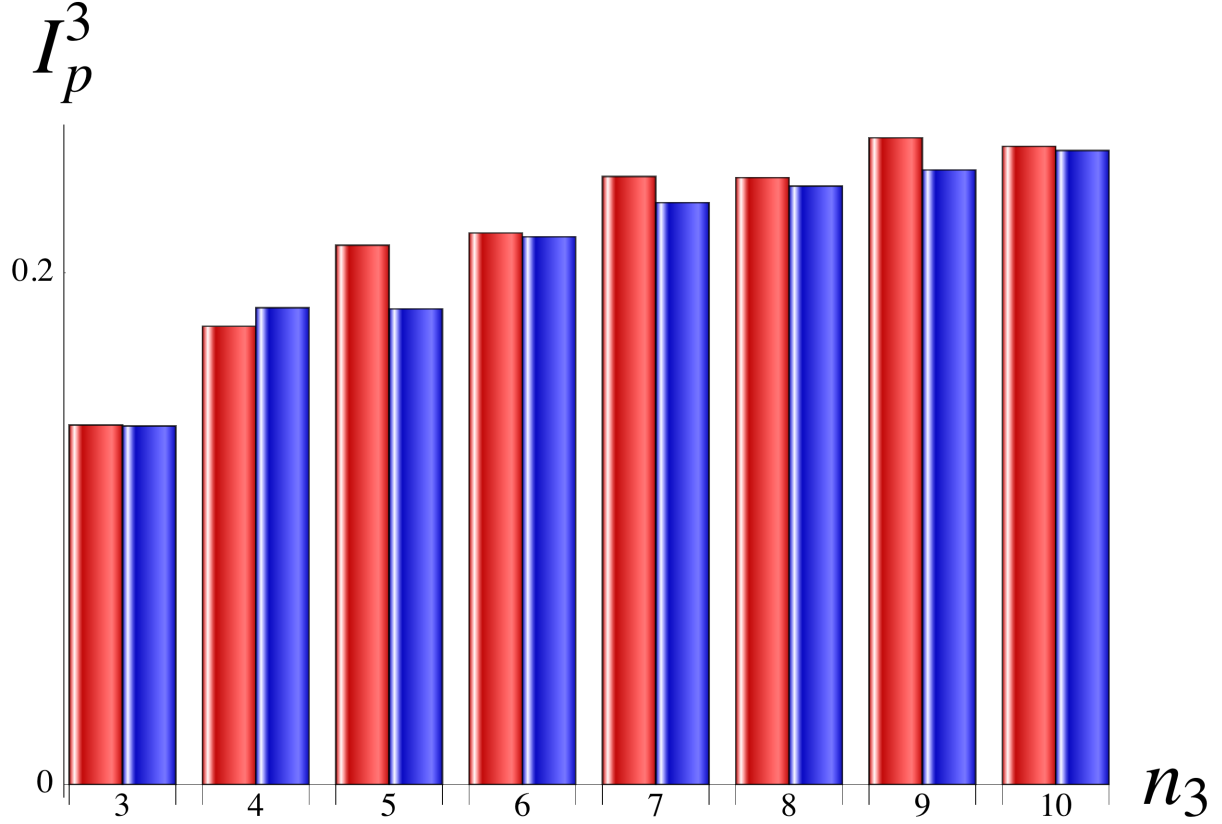


FIG. 8. Higher-order mutual information,  $I_p^3$ , in momentum space for symmetric (red) and antisymmetric (blue) functions, varying  $n_3$  with  $n_1 = 1$ ,  $n_2 = 2$  and  $L = 1$ . Color online.

quantum interference or cross terms between states, that are present in the densities. This type of correlation is distinct from the one due to indistinguishability. The coefficients,  $|c_1|^2 + |c_2|^2 = 1$ , can be varied to change the correlation in the system. We restricted ourselves to real-valued coefficients.

Figure 9 presents values of the third-order and pair mutual informations in position space as  $c_1^2$  is varied from zero to one. We chose to study the particular case of the superposition of

$$\Psi_S(x_1, x_2, x_3) = c_1 \Psi_{1,2,3}(x_1, x_2, x_3) + c_2 \Psi_{4,5,6}(x_1, x_2, x_3). \quad (25)$$

What is clear is that  $I_x^3$  is sensitive to the correlation and attain its maximum at  $c_1^2 = 0.5$ . This corresponds to a balanced superposition state where  $c_1 = c_2 = \frac{1}{\sqrt{2}}$ .

Also interesting in the consideration of these superpositions is that the antisymmetric functions are now more correlated than the symmetric ones. This is opposite to the behavior previously observed for one state.

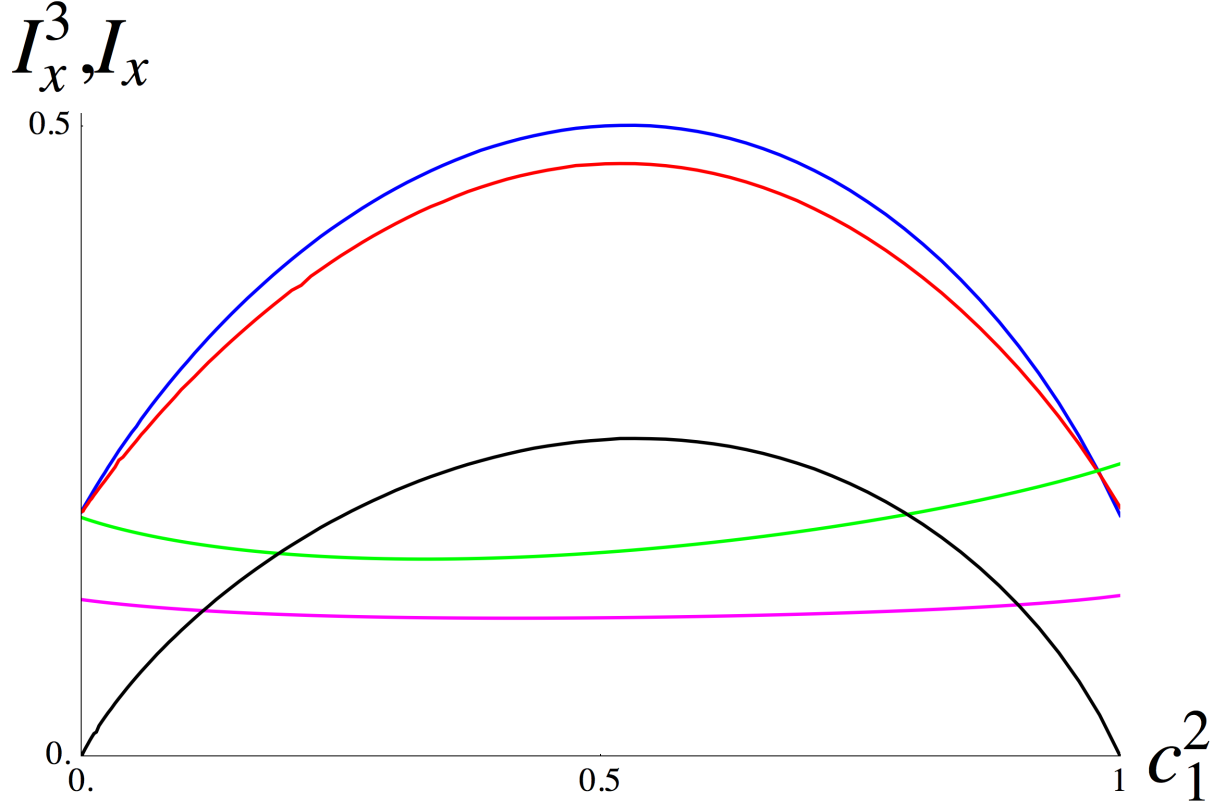


FIG. 9. Higher-order,  $I_x^3$  (symmetric, red), (antisymmetric, blue), and pair,  $I_x$ , mutual informations in position space, from the superposition function,  $\Psi_S(x_1, x_2, x_3)$ , for symmetric (pink) and antisymmetric (green) functions, varying  $c_1^2$ .  $I_x^3$  for the superposition of distinguishable functions,  $\Psi_S^D(x_1, x_2, x_3)$ , (black) is also shown. Color online.

Plots of the pair mutual information are also included in the figure. The results illustrate that this measure is insensitive to the correlation due to the quantum interferences and actually decrease with  $c_1^2$  when one would expect increases due to added correlation.

$I_x^3$  values for superpositions of distinguishable functions,  $\Psi_S^D(x_1, x_2, x_3)$ , (Hartree-like product functions with no symmetrization)

$$\Psi_S^D(x_1, x_2, x_3) = c_1 \psi_1(x_1)\psi_2(x_2)\psi_3(x_3) + c_2 \psi_4(x_1)\psi_5(x_2)\psi_6(x_3), \quad (26)$$

are also presented. One can observe an order in the correlation with the distinguishable functions being the least correlated followed by the symmetric ones and then the antisymmetric ones. This relative ordering holds throughout the range of  $c_1^2$ . Note that  $I_x^3$  is zero when there is no superposition ( $c_1^2$  equal to zero or one) since there is no correlation from indistinguishability in these distinguishable functions.

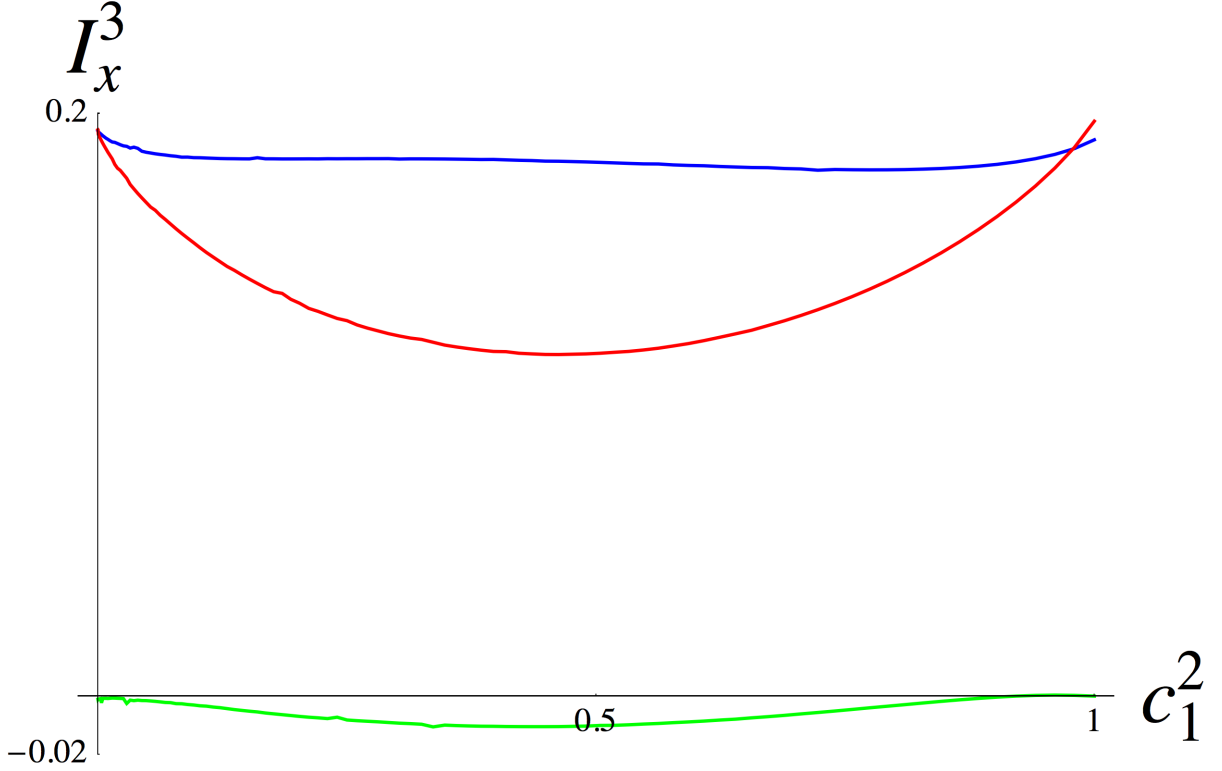


FIG. 10. Higher-order mutual information,  $I_x^3$ , in position space, from the superposition function,  $\Psi_S(x_1, x_2, x_3)$ , without quantum interferences, for symmetric (red) and antisymmetric (blue) functions, varying  $c_1^2$ .  $I_x^3$  for superpositions of the distinguishable functions,  $\Psi_S^D(x_1, x_2, x_3)$ , (green) without quantum interferences, is also shown. Color online.

The higher-order mutual information was further tested by examining the correlation generated from states where the quantum interferences are not included (no  $c_1 c_2$  cross terms in the densities). These results are presented in Figure 10.

It is apparent that the correlation in the antisymmetric functions is now not as sensitive to the value of  $c_1^2$ . This can be contrasted against the behavior in the previous figure and shows that the third-order measure is sensitive to the correlation from the quantum interferences. There is a minimum in the symmetric functions instead of the maximum in the previous figure. However, the antisymmetric functions are more correlated than the symmetric ones ( $0 < c_1^2 < 1$ ) as in the previous figure where quantum interferences are included. When  $c_1^2$  is equal to zero or one, the symmetric functions are more correlated.

Results from the distinguishable functions show negative values for the third-order measure and can be contrasted to the positive values which occur when indistinguishability is

imposed, or in the previous figure when quantum interferences are included. This suggests that the positivity or negativity of the third-order mutual information depends on physical constraints imposed on the system. Furthermore, the minimum where  $I_x^3$  is maximally negative, occurs when  $c_1 = c_2 = \frac{1}{\sqrt{2}}$ .

The interpretation in momentum space is less clear and the plots are not presented. The reason is that the quantum interferences in momentum space do not contribute to a large extent in the overall correlation. It is now the mutual information between pairs which exhibit maximal correlation at the balanced superposition state. On the other hand, the third-order measures exhibit minima instead of the maxima seen in the previous figures. Similar to position space, the distinguishable functions without quantum interferences yield negative values.

## VII. CONCLUSIONS

Higher-order mutual information is used to quantify and study the higher-order statistical correlation present in a system of three spinless non-interacting quantum particles in a unidimensional box, in position and in momentum space. The statistical correlation in these systems arises from the indistinguishability requirements on the wave function. The results show that the magnitude of the higher-order mutual information is larger for the symmetric wave functions in comparison to the antisymmetric ones with the same quantum numbers. This is in contrast to other three-variable measures and the two-variable (pair) mutual information where the antisymmetric functions are more correlated. It is also distinct from similar two-particle systems where the antisymmetric functions are in general more correlated. Indeed, more particles lead to a different behavior<sup>45</sup>. The utility of higher-order mutual information as a correlation measure is explored by considering a superposition of states where there is correlation due to quantum interferences. We observe that the magnitude of the higher-order mutual information is sensitive to the superposition coefficients with the maximum value attained for the balanced superposition state. This provides evidence that the magnitude can be used as a measure of correlation strength. Furthermore, the inclusion of superposition induces the antisymmetric functions to now be more correlated than the symmetric ones, with both being more correlated than distinguishable functions. The pair mutual information is less sensitive to the correlations arising from the

quantum interferences due to the use of reduced densities in its definition. Higher-order mutual information arising from superpositions of distinguishable functions without quantum interferences is negative-valued. This is in contrast to the positive values obtained when the quantum interferences are included, and to the results from superpositions of symmetric and antisymmetric functions. These results suggest a dependence of the sign of higher-order mutual information on physical constraints in these systems.

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